Data Assimilation and Uncertainty Management of Large-dimensional Dynamics models

CASIS Workshop 2016

Xiao Chen, Charles Tong, Josh White, and Christina Morency

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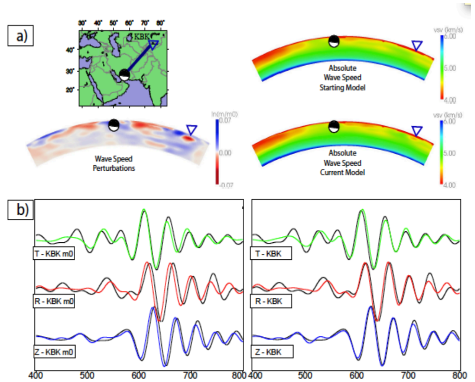
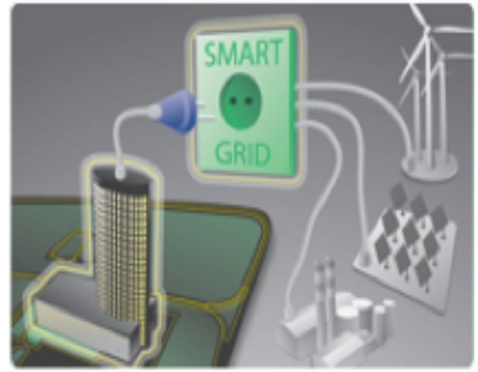
Several real-world applications require efficient and robust capabilities to recover an unknown and complex field from noisy measurements

Seismic inversion



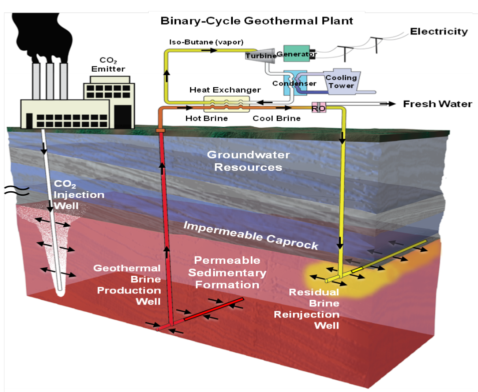
Target: Wave speed field
Data: waveform measurements

Power grid management



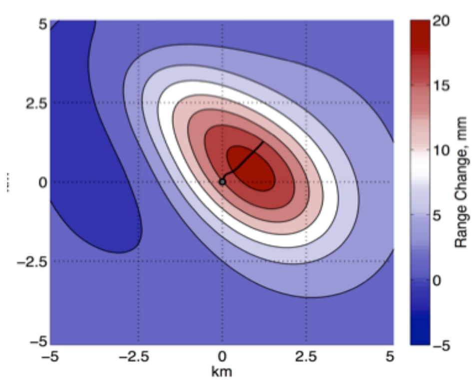
Target: network loads (at nodes)
Data: measurement of 'dispatch'

Reservoir simulation



Target: permeability field
Data: pressures from sensors

SubTER Initiative

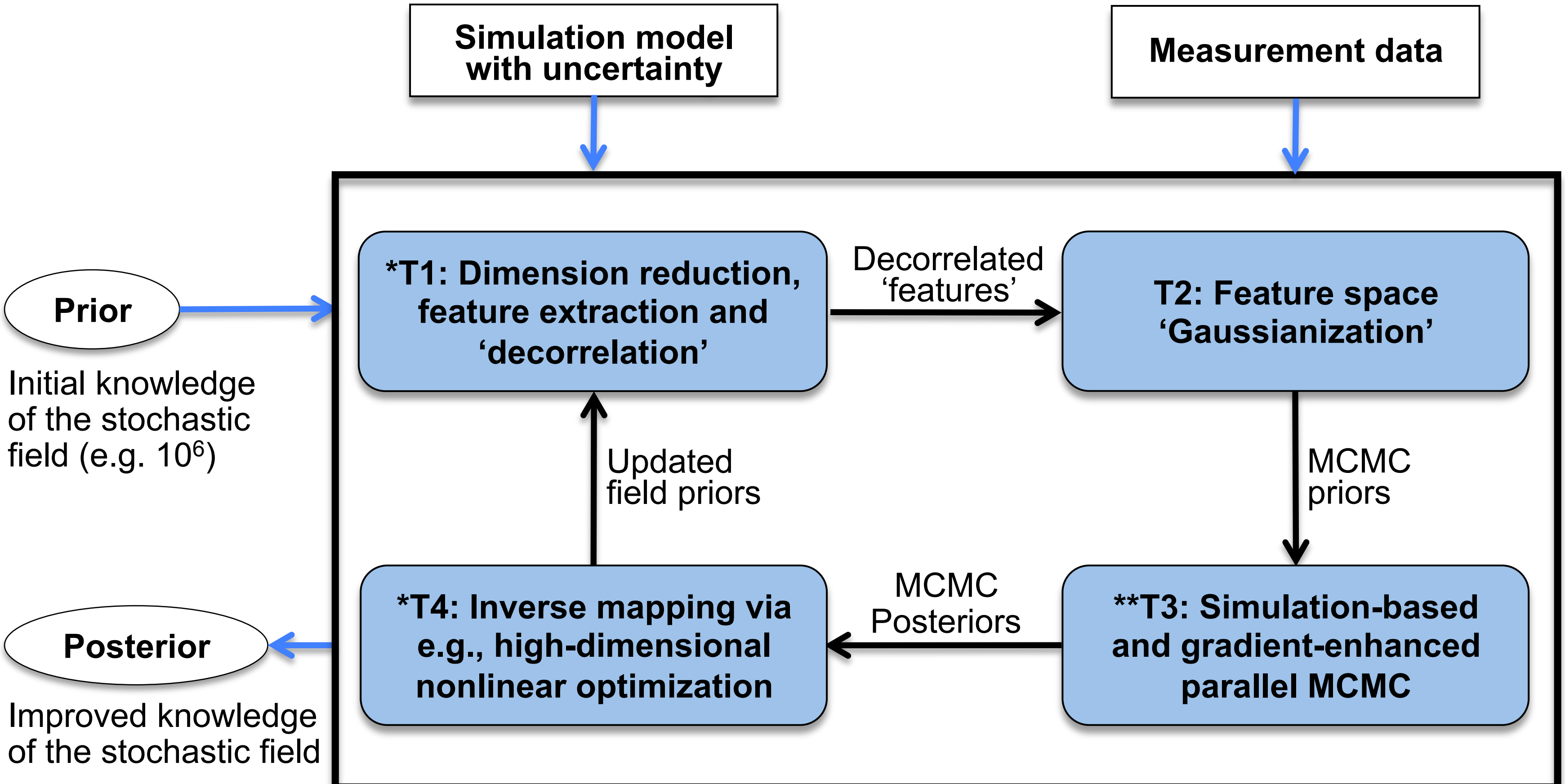


Target: subsurface structure
Data: surface deformation

Common characteristics:

- **Target:** spatial random field
  - High dimensionality
  - Nonlinearly correlated
  - Non-Gaussian
- **Data** (measurements)
  - Noisy and sparse
- **Simulation-based**
  - Computationally intensive
  - Models have uncertainties
- **Need:**
  - Accurate inversion for credible decision making
  - Fast solution for timely analysis

Our vision is to build an innovative computational capability for high-dimensional statistical inversion without Gaussian/linearity assumptions



MCMC = Markov Chain Monte Carlo
* = HPC intensive

Kernel principal component analysis (KPCA) based PDE constrained nonlinear optimal control is outlined as the following

$$\min J\left(\mathbf{y}\left(\mathbf{x}\right)\right)$$

A cost functional one needs to minimize

$$M\left(\mathbf{y}\left(\mathbf{x}\right)\right)=0$$

Subject to a nonlinear simulation model as a constraint

$$f\left(\mathbf{y},\mathbf{x}\right)=0$$

Continuous parameterization: parameters **y** and normal random variables **x** satisfy an implicit equation derived by a kernel PCA

$$\nabla_{\mathbf{x}} J=\left(\frac{d\mathbf{y}}{d\mathbf{x}}\right)^{\mathrm{T}}\nabla_{\mathbf{y}} J$$

The gradient of J to **x** by a adjoint operator on a gradient of J to **y** computed by the *adjoint* model

$$\left(\frac{d\mathbf{y}}{d\mathbf{x}}\right)^{T}$$

The *adjoint* operator is computed by an automatic differentiation

The adjoint-based linear elasticity inversion problem is described as the following

$$\nabla \cdot \left((\lambda \nabla \cdot u) \mathbf{I} + \mu \left(\nabla u + \nabla u^{\mathrm{T}} \right) \right) = 0 \text{ in } \Omega$$
$$\left((\lambda \nabla \cdot u) \mathbf{I} + \mu \left(\nabla u + \nabla u^{\mathrm{T}} \right) \right) \cdot n = h \text{ on } \Gamma_h$$
$$u = r \text{ on } \Gamma_r$$

Forward model

$$\nabla \cdot \left((\lambda \nabla \cdot w) \mathbf{I} + \mu \left(\nabla w + \nabla w^{\mathrm{T}} \right) \right) = -\left(u - u^m \right) \text{ in } \Omega$$
$$\left((\lambda \nabla \cdot w) \mathbf{I} + \mu \left(\nabla w + \nabla w^{\mathrm{T}} \right) \right) \cdot n = 0 \text{ on } \Gamma_h$$
$$w = 0 \text{ on } \Gamma_r$$

Adjoint model

$$\begin{aligned} J\left(y\left(x\right)\right) &= J_b\left(x\right) + \frac{1}{2} \parallel u - u^m \parallel_\Omega^2 \\ &= J_b\left(x\right) + J_o\left(y\left(x\right)\right) \end{aligned}$$

Cost function

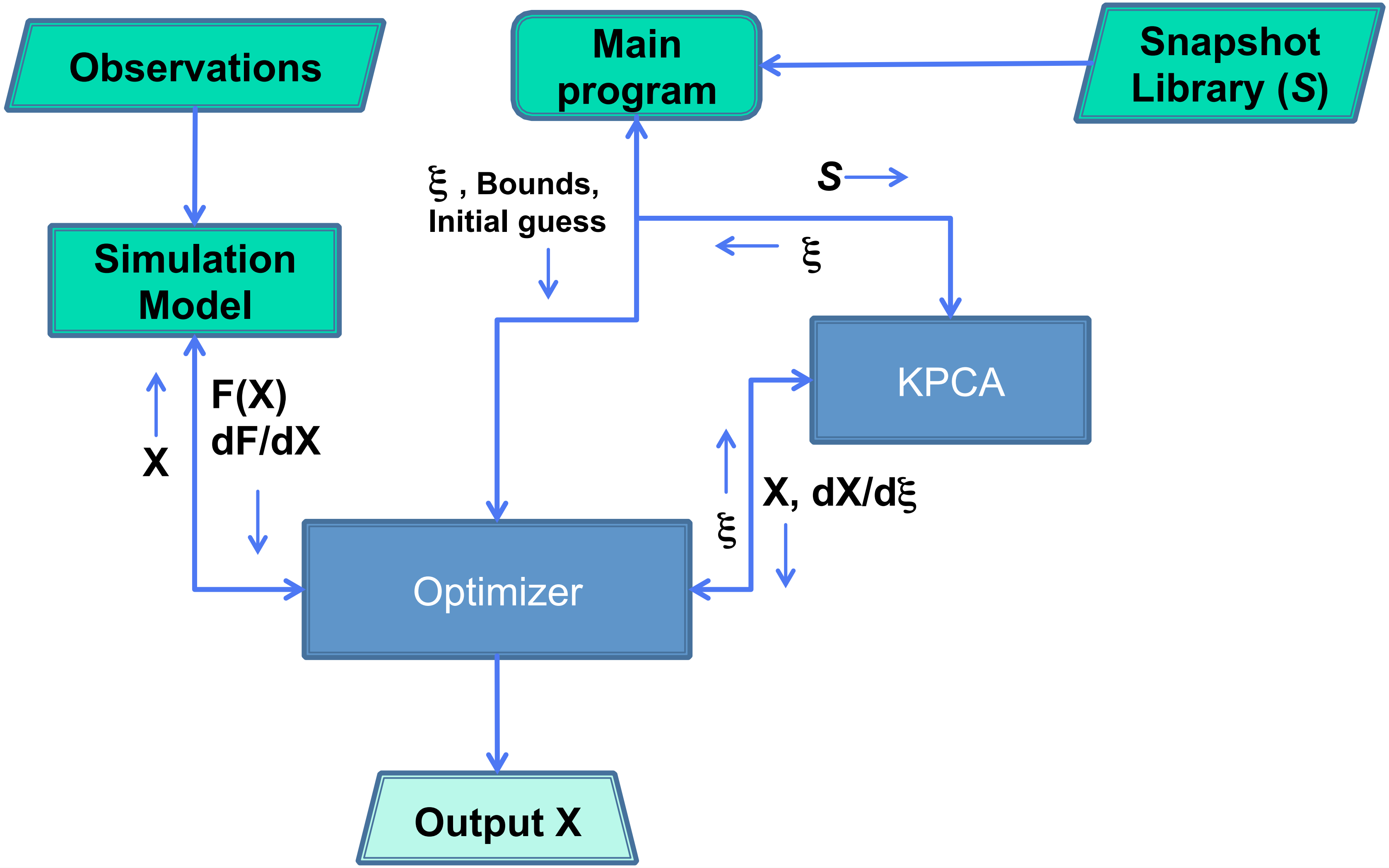
$$\nabla_{\mathbf{y}} J_o = g = \begin{bmatrix} g_1 & g_2 & g_3 \end{bmatrix}^{\mathrm{T}}$$

$$\begin{aligned} g_{1i} &= A_1\left(w_h, u_h; \phi_i\right) \\ g_{2i} &= A_2\left(w_h, u_h; \phi_i\right) \\ g_{3i} &= -\left(w_h, \phi_i\right)_{\Gamma_h} = -\int_\Gamma w_h \cdot \phi_i \mathrm{d}\Gamma \end{aligned}$$

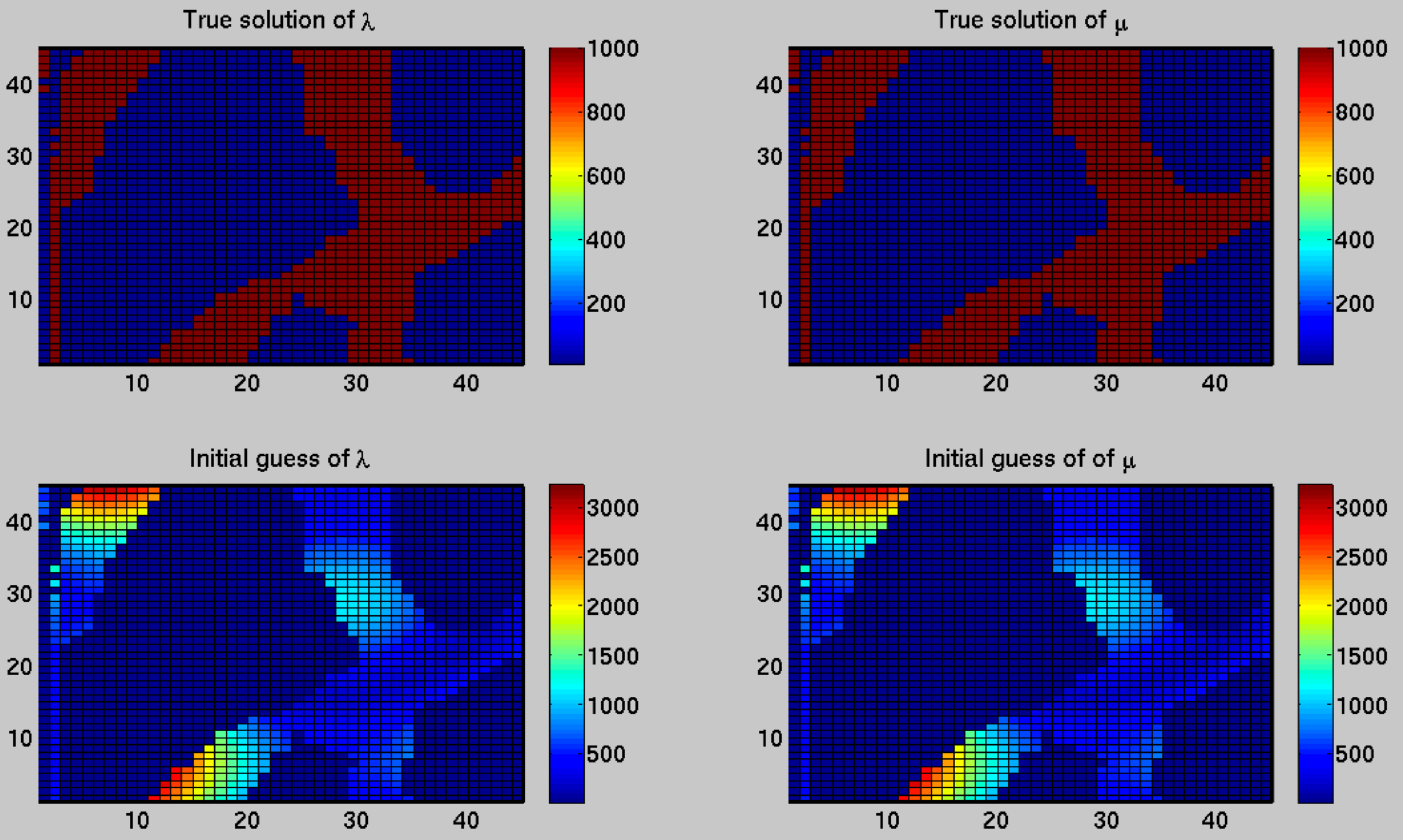
$$\begin{aligned} A_1\left(w_h, u_h; \phi_i\right) &= \int_\Omega \frac{\phi_i}{2} \left(\nabla w_h + \nabla {w_h}^{\mathrm{T}} \right) : \left(\nabla u_h + \nabla {u_h}^{\mathrm{T}} \right) \mathrm{d}\Omega \\ A_2\left(w_h, u_h; \phi_i\right) &= \int_\Omega \phi_i \left(\nabla \cdot w_h \right) : \left(\nabla \cdot u \right) \mathrm{d}\Omega \end{aligned}$$

Gradient calculation

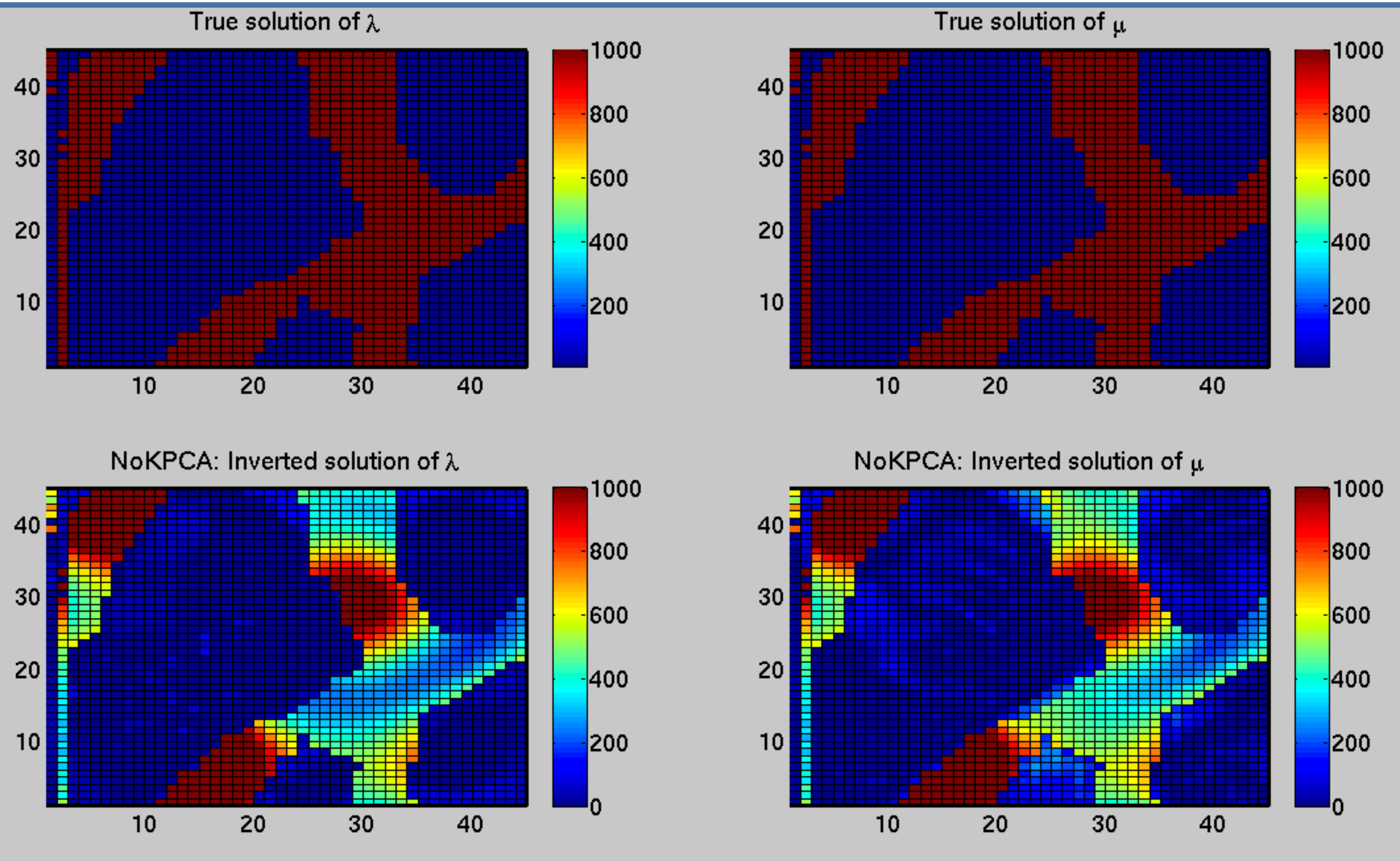
The flowchart of the framework for coupling nonlinear optimal control with kernel PCA is described as the following



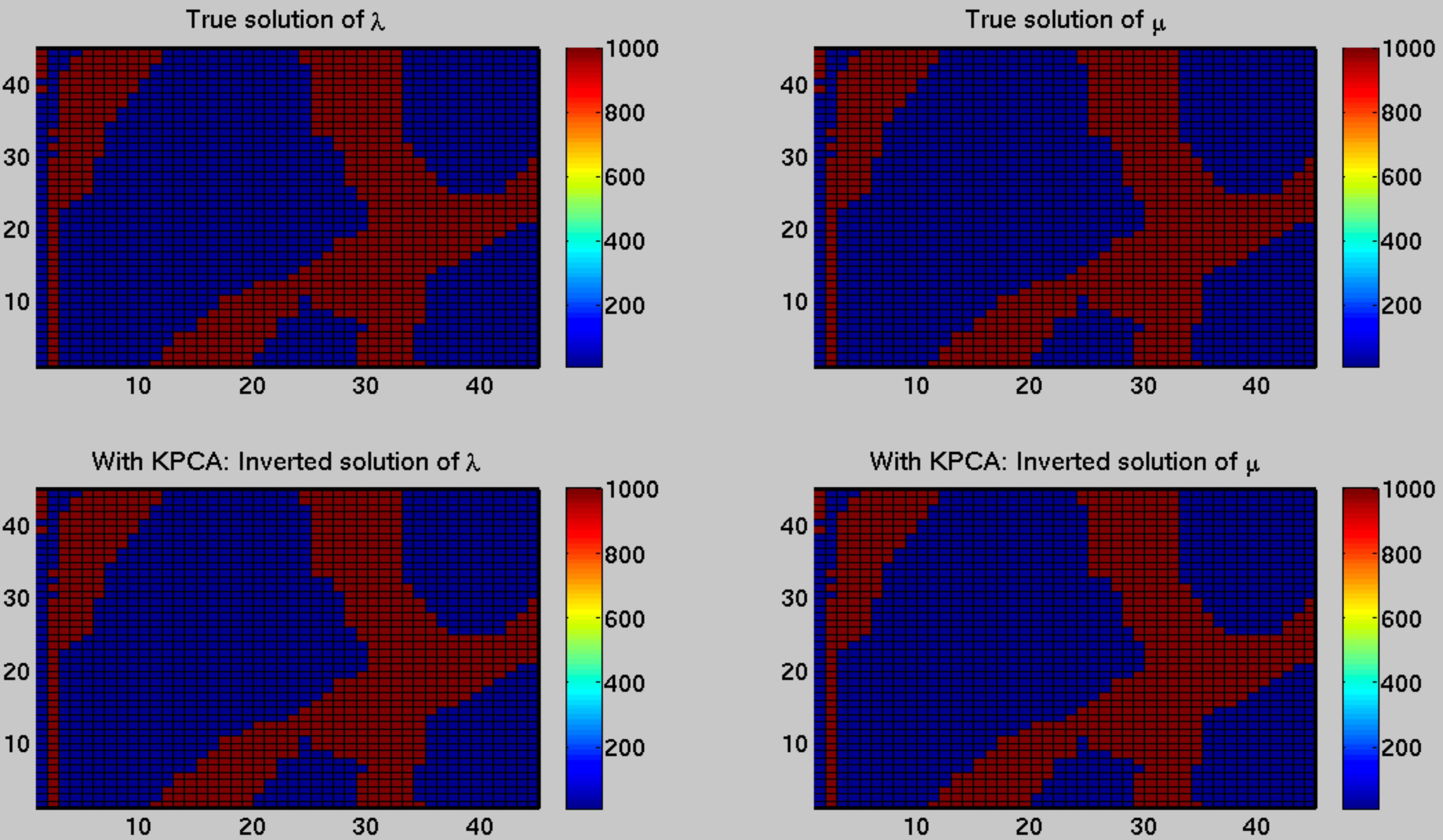
We perturb a pre-selected channelized material property field with 10 types of trigonometric functions to generate 200 snapshots then use one as true solution and snapshots average as an initial guess of the true solution



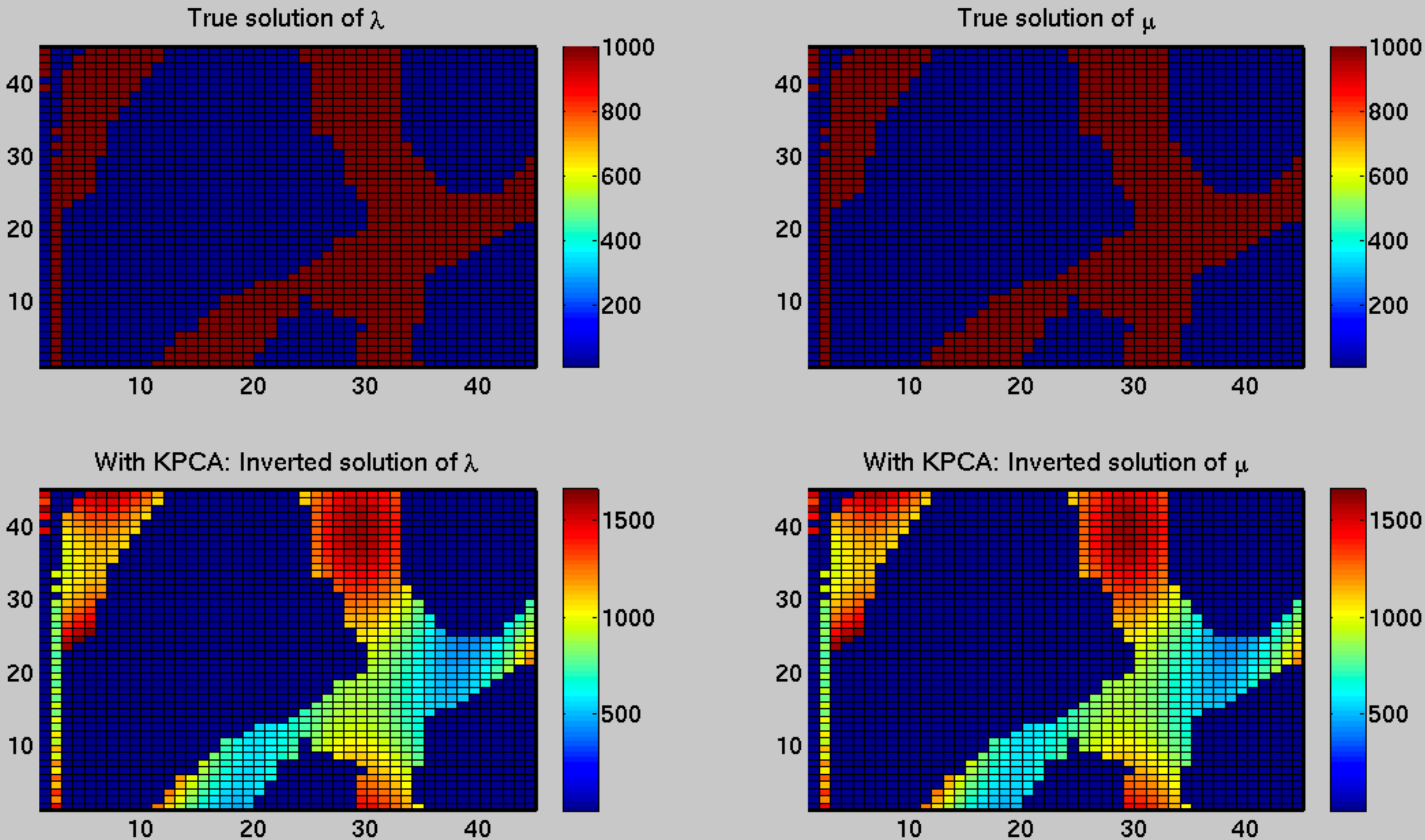
We solve the linear elasticity inversion problem by L-BFGS based non-linear optimization without the use of either linear PCA or kernel PCA



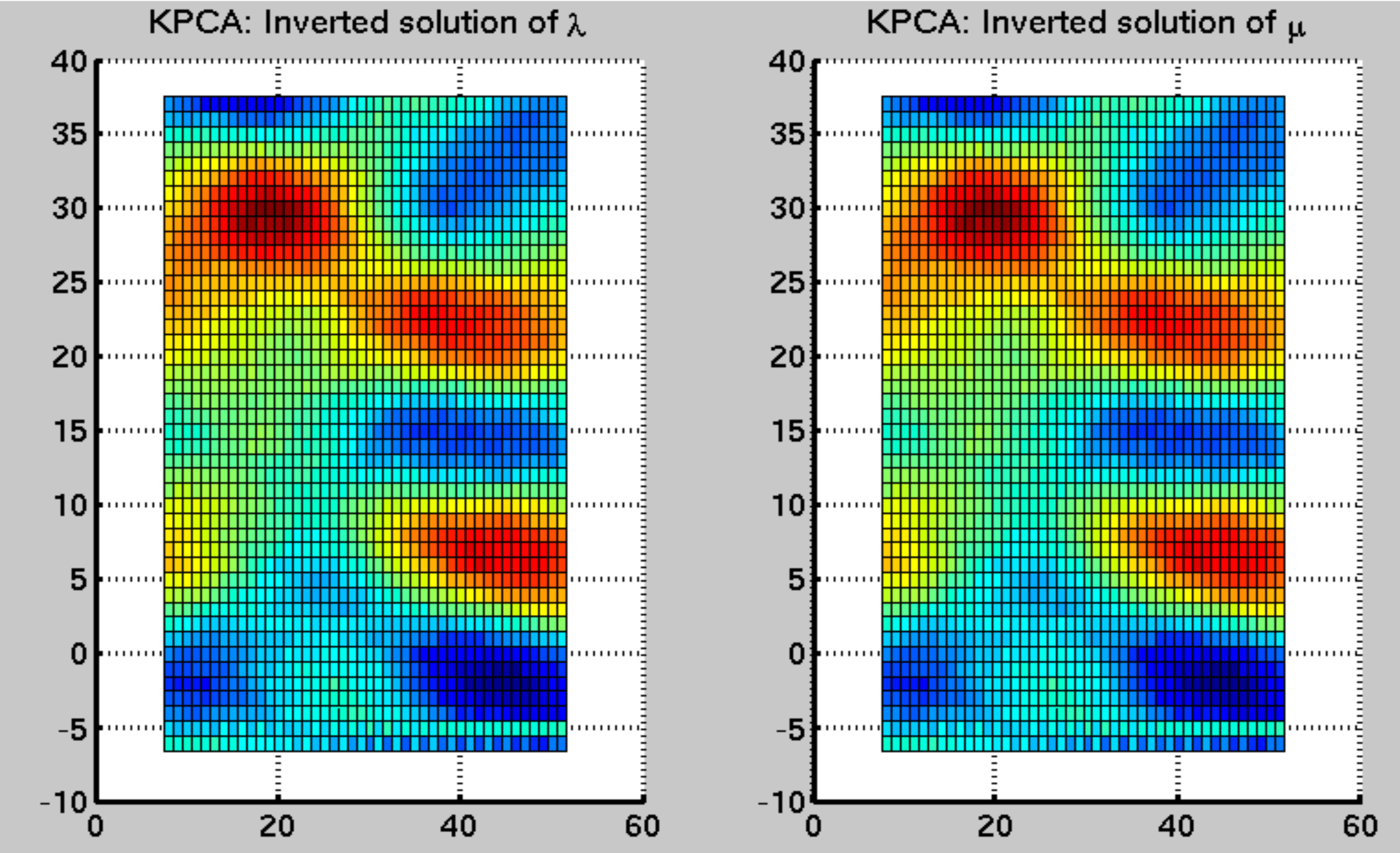
We then solve the linear elasticity inversion using L-BFGS coupled with either linear PCA or kernel PCA by choosing 10 leading principle components



We also solve the linear elasticity inversion using LBFGS coupled with either linear PCA or kernel PCA by choosing 9 leading principle components



Typical realizations obtained with kernel PCA of order 1 (linear PCA) are plotted as the following



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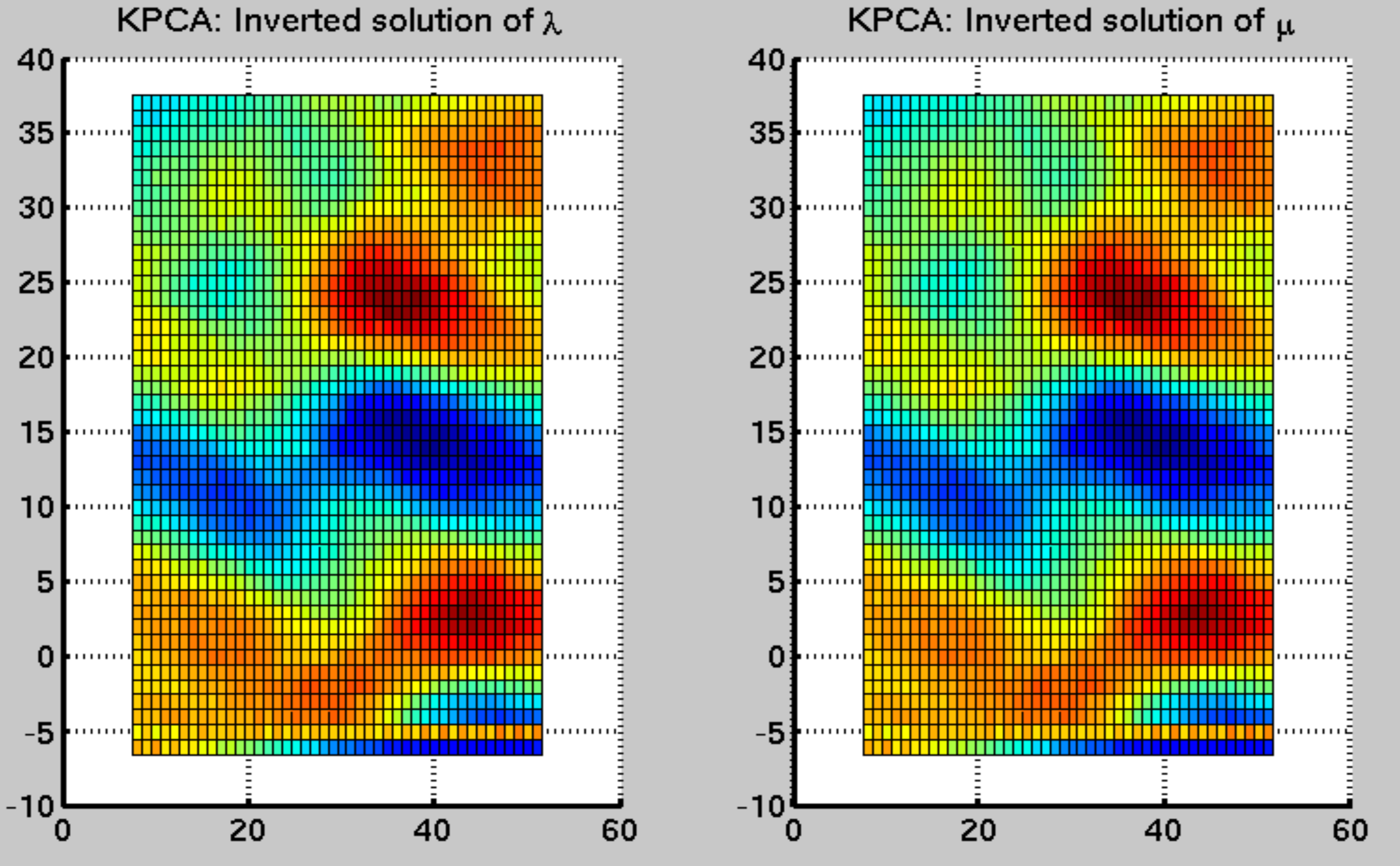

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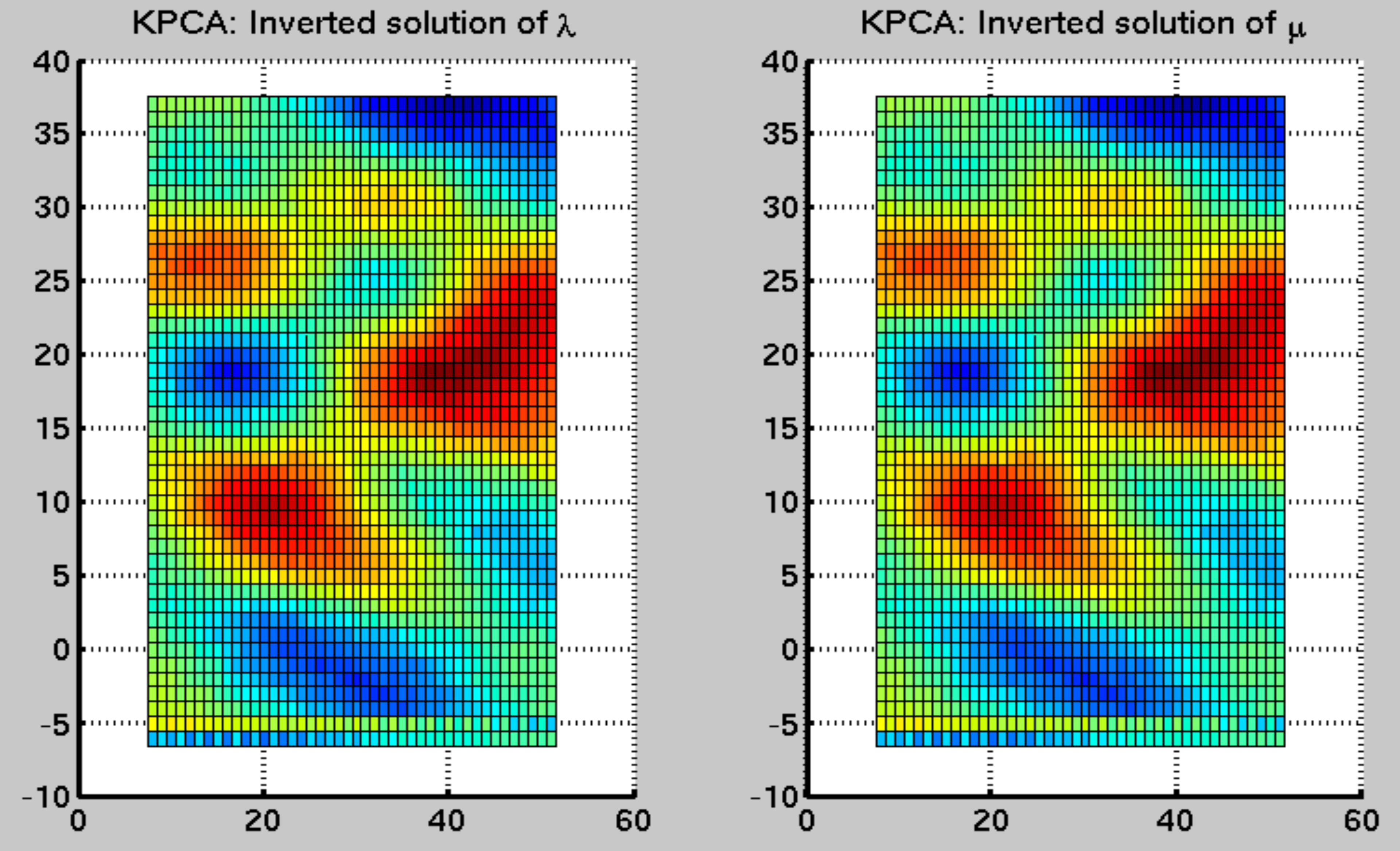
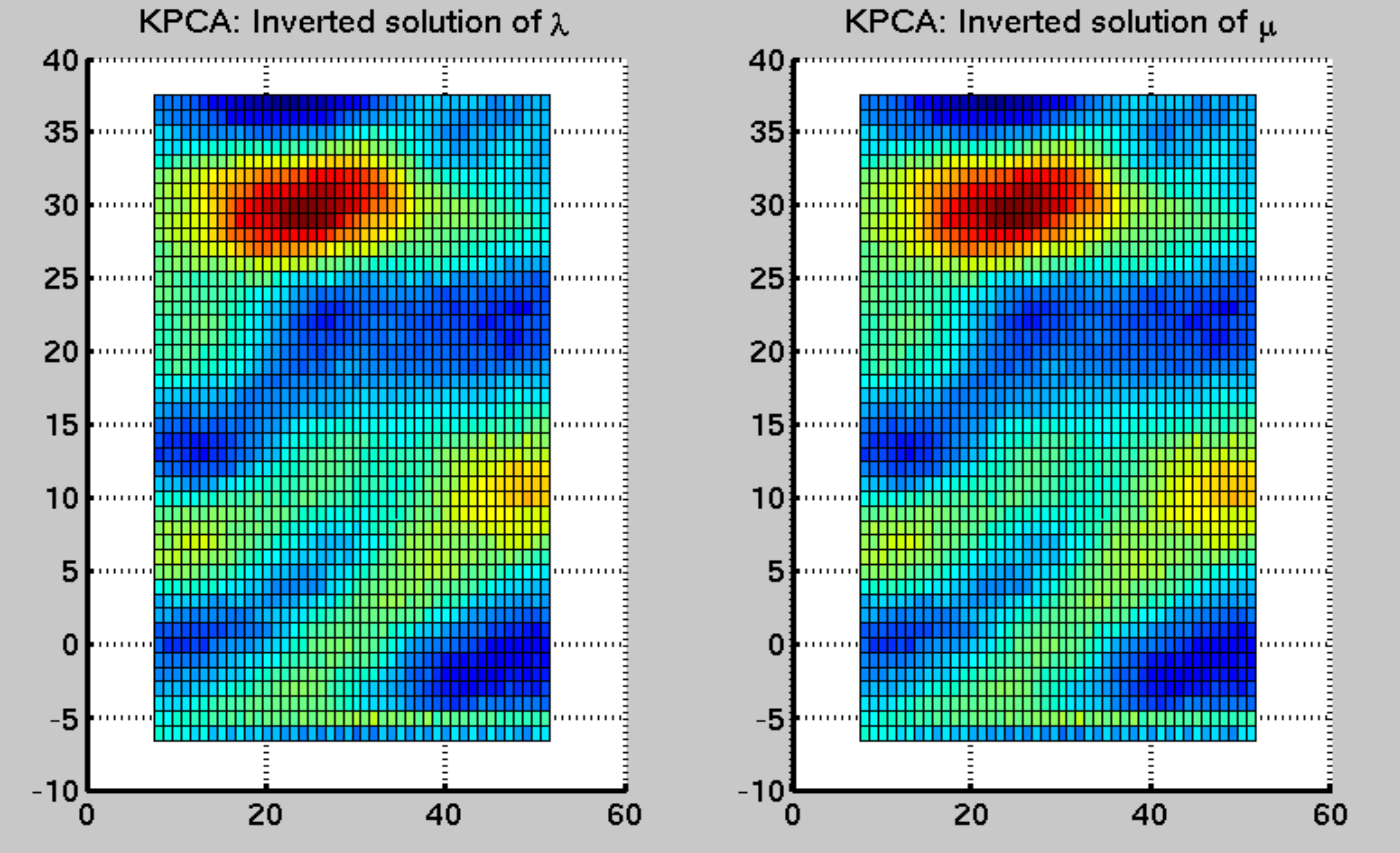
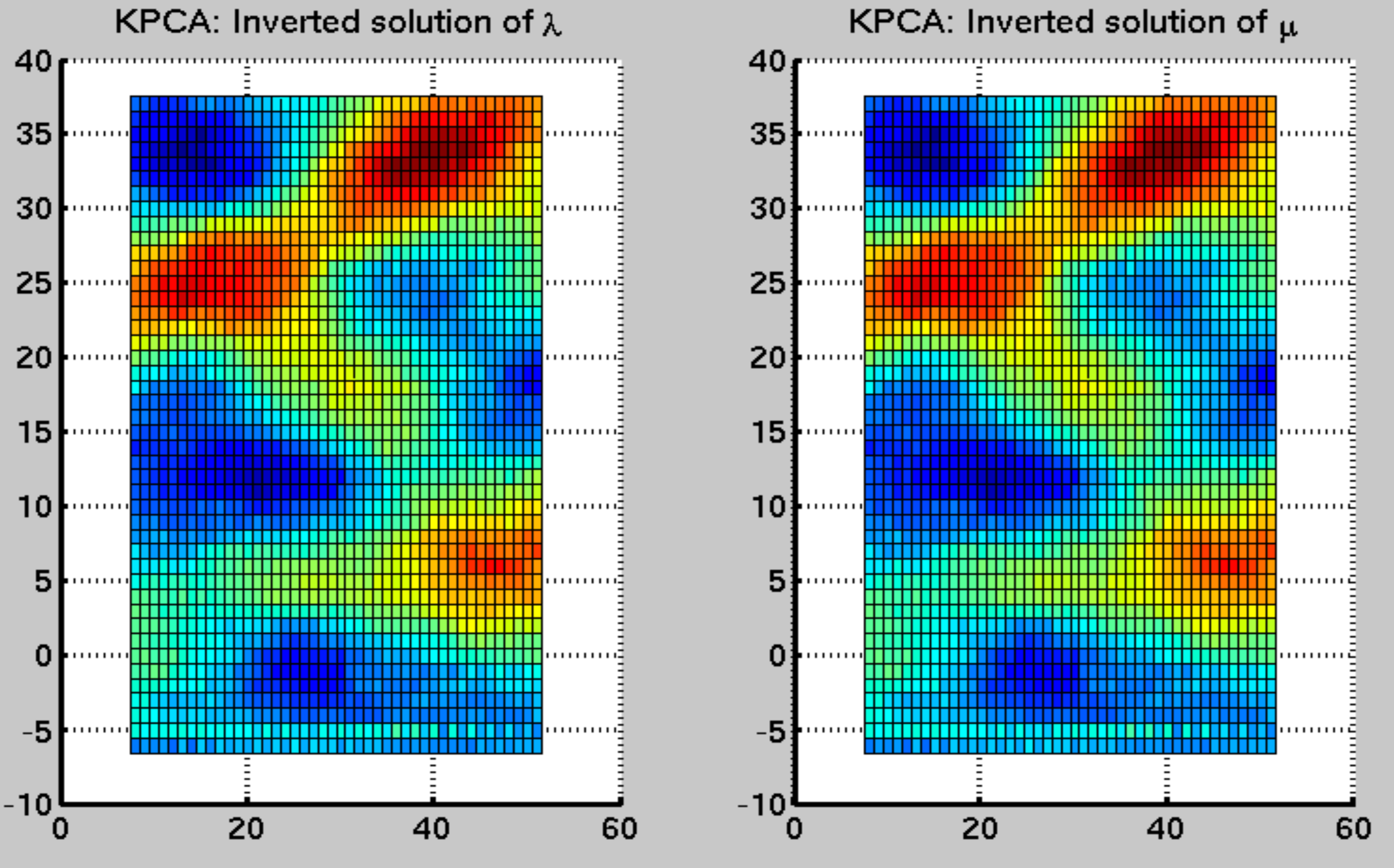


Typical realizations obtained with kernel PCA of order 3 are plotted as the following



Typical realizations obtained with kernel PCA of order 3 are plotted as the following



Typical realizations obtained with kernel PCA of order 3 are plotted as the following